Lattice-matched Cu2ZnSnS4/CeO2 solar cell with open circuit voltage boost

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Lattice-matched Cu_2ZnSnS_4/CeO_2 solar cell with open circuit voltage boost

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We propose and test experimentally CeO_2 as a novel buffer layer material in pure-sulfide CZTS solar cells. The major advantage of CeO_2 is its nearly perfect lattice match with CZTS (0.4%), in contrast to CdS which has a large lattice mismatch with CZTS (7%). CeO_2 is a non-toxic compound that is already used in the fields of catalysis and solid oxide fuel cells. Ce is more earth-abundant than Sn and about as earth-abundant as Cu and Zn (source: U.S. Geological Survey Fact Sheet 087-02).

In this work we demonstrate that CeO_2 can be easily grown on CZTS by chemical bath deposition at low temperature, showing good surface coverage (Figure 1), low spurious phase content, and a nearly optimal band alignment with CZTS as measured by x-ray photoemission spectroscopy.

We then make a first attempt to include CeO_2 in the CZTS solar cell architecture by inserting a thin CeO_2 layer between CZTS and the usual CdS buffer to check its passivation properties on the CZTS surface. The result (over four solar cell batches up to 7% efficiency) is a reproducible open circuit voltage boost compared to the baseline case with a pure CdS buffer layer (Figure 2). The efficiency is also improved in three batches out of four. We argue that this is due to formation of a less defective heterointerface with a lower recombination velocity. By looking at the band structure and electronic properties of the CeO_2 from theory, we discuss why CeO_2 can be an excellent surface passivation layer for CZTS but cannot be used a stand-alone buffer layer in CZTS solar cells.

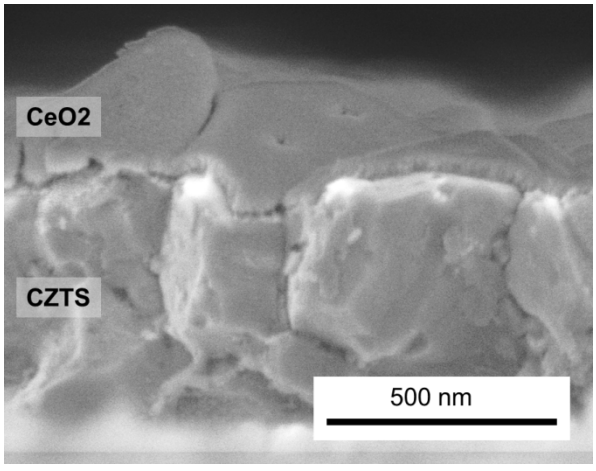

Figure 1: SEM image of CeO_2 grown on CZTS

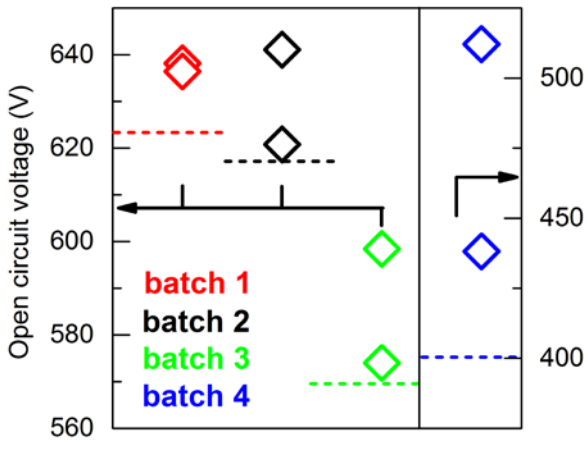

Figure 2: Open circuit voltage of CZTS solar cells with a CeO_2 interlayer (diamond data points) compared to the reference CdS-buffer cells (dashed lines) in the same batch.